

The no-core shell model with general radial bases

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Abstract. Calculations in the *ab initio* no-core shell model (NCSM) have conventionally been carried out using the harmonic-oscillator many-body basis. However, the rapid falloff (Gaussian asymptotics) of the oscillator functions at large radius makes them poorly suited for the description of the asymptotic properties of the nuclear wavefunction. We establish the foundations for carrying out no-core configuration interaction (NCCI) calculations using a basis built from general radial functions and discuss some of the considerations which enter into using such a basis. In particular, we consider the Coulomb-Sturmian basis, which provides a complete set of functions with a realistic (exponential) radial falloff.

1. Introduction

Significant advances presently are being made towards one of the basic goals of nuclear theory, namely, an *ab initio* understanding of the nucleus directly as a system of interacting protons and neutrons. Nuclear interactions motivated by quantum chromodynamics are being developed, via effective field theory methods [1, 2], to provide an underlying Hamiltonian. It is then necessary to solve the many-body problem for this Hamiltonian, obtaining nuclear eigenstates and predictions for observables. In no-core configuration interaction (NCCI) approaches such as the no-core shell model (NCSM) [3], the eigenproblem is formulated as a matrix diagonalization problem, in which the Hamiltonian matrix is represented with respect to a basis of antisymmetrized products of single-particle states, for the full A -body system of nucleons.

Actual NCCI calculations must be carried out in a finite, truncated space. The challenge is to reach a reasonable approximation of the converged results which would be achieved in the full, untruncated space for the many-body system. The success of the calculation is determined by the rate of convergence of calculated observables (*e.g.*, energies, radii, and electromagnetic moments and transition strengths) with increasing basis size and the ability to reliably extrapolate these results to the full, untruncated many-body space [4, 5]. Convergence rates are sensitive to the choice of single-particle states from which the many-body basis is constructed, as well as the truncation scheme used for the many-body basis.

In practice, such calculations have been based almost exclusively on a harmonic oscillator basis. It is worth recalling the special characteristics of this basis which make it particularly convenient for use in the nuclear many-body problem:

(1) An exact factorization of center-of-mass and intrinsic wavefunctions is obtained in many-body calculations when the oscillator basis is used in conjunction with the N_{max} truncation scheme, which is based on the total number of oscillator quanta. Thus, precise removal of, or correction for, spurious center-of-mass contributions to the dynamics is possible.

(2) Matrix elements of the nucleon-nucleon two-body interaction are naturally formulated in the relative oscillator basis. These matrix elements can easily be transformed to the two-body oscillator basis, of functions $\Psi_{n_1 l_1}(\mathbf{r}_1)\Psi_{n_2 l_2}(\mathbf{r}_2)$, by the Moshinsky transformation [6]. The simplicity of this transformation is lost with any other single-particle basis.

(3) The oscillator functions constitute a complete *discrete* basis for square-integrable functions. Many alternative bases, such as the eigenfunctions of the Schrödinger equation for a *finite-depth* potential such as the Woods-Saxon potential, do not provide this convenience, since for these bases a continuum of unbound single-particle states is needed for completeness.

However, there are also significant motivations for moving beyond the oscillator basis for the nuclear many-body problem [7]. The classic physical limitation of the oscillator basis, for application to the nuclear problem, lies in the Gaussian falloff ($\propto e^{-\alpha r^2}$) at large distance r . In contrast, for particles bound by a finite-range force, the actual asymptotics are exponential ($\propto e^{-\beta r}$). This mismatch in asymptotics, *i.e.*, the wavefunction tails, between the expansion basis and the physical system imposes a serious handicap on the convergence of calculations with increasing basis size. The problem is especially significant for observables, such as the root-mean-square radius or $E2$ strengths, which are sensitive to the large- r properties of the nuclear wavefunctions.

Here we consider an alternative basis for NCCI calculations, built from Coulomb-Sturmian functions [8, 9].¹ Although we focus on the Coulomb-Sturmian basis, many of the considerations addressed here are more broadly applicable to alternative single-particle bases for the NCCI problem. First, the procedures and results necessary for using the Coulomb-Sturmian basis for nuclear many-body calculations are outlined (section 2). Then, illustrative calculations for ${}^6\text{Li}$ are discussed (section 3). An expanded discussion may be found in [10].

2. Coulomb-Sturmian basis

The Coulomb-Sturmian functions [8, 9, 11], have previously been applied to few-body problems in atomic [8, 11–13] and hadronic [14–16] physics. They constitute a complete, discrete, orthogonal set of square-integrable functions, while also possessing realistic exponential asymptotics appropriate to the nuclear problem. The functions on \mathbb{R}^3 are given by $\Lambda_{nlm}(\mathbf{r}) = S_{nl}(r)Y_{lm}(\hat{\mathbf{r}})/r$, with radial wave function

$$S_{nl}(b; r) \propto (2r/b)^{l+1} L_n^{2l+2}(2r/b) e^{-r/b}, \quad (1)$$

where the L_n^α are generalized Laguerre polynomials, the Y_{lm} are spherical harmonics, n is the radial or node quantum number, l and m are the orbital angular momentum and its z -projection, and b is a radial scale parameter, analogous to the oscillator length parameter for the harmonic oscillator functions. The first several Coulomb-Sturmian radial functions, for $l = 0$, are plotted in figure 1(a). The radial functions for the harmonic oscillator are shown for comparison in figure 1(b).

Many-body calculations with the Coulomb-Sturmian basis can make use of the existing computational framework for NCCI calculations, but starting from the two-body matrix elements of the Hamiltonian in this new basis. The change of basis transformation has the form

$$\langle \bar{c}\bar{d}; J | V | \bar{a}\bar{b}; J \rangle = \sum_{abcd} \langle a|\bar{a} \rangle \langle b|\bar{b} \rangle \langle c|\bar{c} \rangle \langle d|\bar{d} \rangle \langle cd; J | V | ab; J \rangle, \quad (2)$$

¹ Since the Coulomb-Sturmian single-particle states arise [8] as solutions to a general Sturm-Liouville equation, rather than a Schrödinger equation or Hartree-Fock problem, it may be noted that they do not physically correspond to “shells” in the conventional sense. That is, they are not naturally interpreted as orbitals for independent-particle motion in some mean-field potential describing the zeroth-order dynamics of the system. Therefore, we will use the more inclusive term *configuration interaction*, rather than specifically *shell model*.

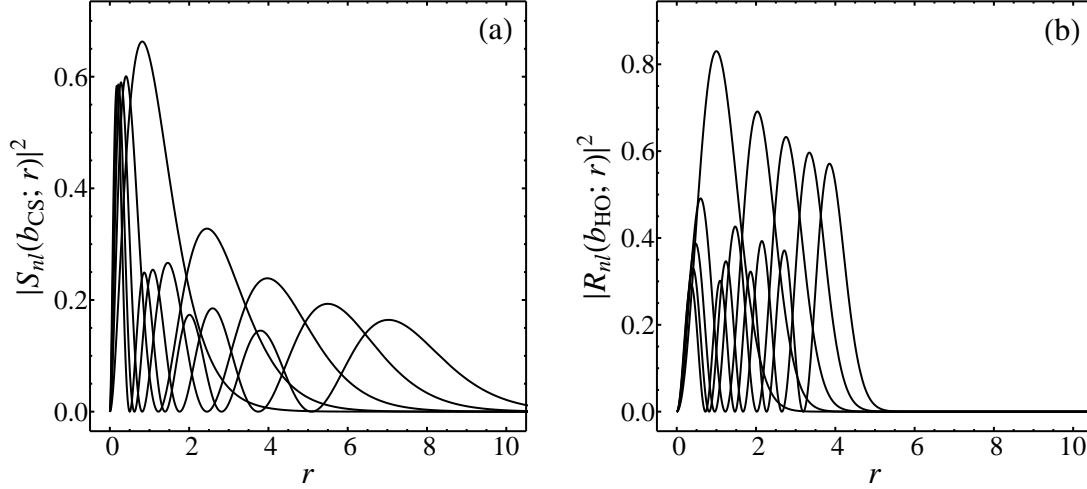


Figure 1. Radial functions for the (a) Coulomb-Sturmian and (b) harmonic oscillator bases, for $l = 0$. The first five functions ($0 \leq n \leq 4$) are shown in each case.

where in this expression we label single-particle orbitals for the oscillator basis by unbarred symbols $a = (n_a l_a j_a)$, $b = (n_b l_b j_b)$, *etc.*, and those for the Coulomb-Sturmian basis by barred symbols $\bar{a} = (\bar{n}_a \bar{l}_a \bar{j}_a)$, $\bar{b} = (\bar{n}_b \bar{l}_b \bar{j}_b)$, *etc.* The coefficients $\langle a | \bar{a} \rangle$ required for the transformation are given by the overlaps of the harmonic oscillator and Coulomb-Sturmian radial wavefunctions, that is, $\langle a | \bar{a} \rangle = \langle R_{n_a l_a} | S_{\bar{n}_a \bar{l}_a} \rangle \delta_{(l_a j_a)(\bar{l}_a \bar{j}_a)}$, where $\langle R_{nl} | S_{\bar{n}l} \rangle = \int_0^\infty dr R_{nl}(b_{HO}; r) S_{\bar{n}l}(b_l; r)$. The length parameter for Coulomb-Sturmian and oscillator functions may be chosen independently in this transformation.²

For actual calculation of the transformed matrix elements, the infinite sums over single-particle states appearing in the transformation (2) must be truncated, limited in practice by the available set of oscillator-basis matrix elements. In a single-particle space truncated by number of oscillator quanta, to $N \leq N_{\text{cut}}$, the sum appearing in (2) becomes $\sum_{abcd}^{N_a, N_b, N_c, N_d \leq N_{\text{cut}}}$. The question is whether or not we can practically include enough oscillator shells in the sum to achieve sufficient accuracy for the many-body calculation. Notice that the comparatively longer tails of the Coulomb-Sturmian functions [figure 1(a)] imply that they will require oscillator functions of significantly higher n [figure 1(b)] for their expansion. One might therefore ask now what we have gained by changing to an alternative radial basis, if we must still expand the new basis in terms of high- n oscillator basis functions. The essential point is that we need only carry out the expansion at the *two-body* level, where it is still tractable, to encode the information needed for treatment of the *A-body* problem in the new basis.

Although the truncated transformation (2) is found to suffice for the matrix elements of the nucleon-nucleon interaction, with $N_{\text{cut}} \lesssim 13$ (section 3), the matrix elements of the kinetic energy are significantly more sensitive to the shell cutoff in the transformation. These matrix elements may instead be evaluated directly, making use of the particularly simple form of the kinetic energy operator. The NCSM intrinsic Hamiltonian has the form $H = T_{\text{rel}} + V_{NN}$, where

² Moreover, it is of practical importance to note that orthogonality of Coulomb-Sturmian wavefunctions $\Lambda_{nlm}(\mathbf{r})$ with *different* l quantum numbers is enforced by the $Y_{lm}(\hat{\mathbf{r}})$ factor, regardless of the radial wavefunction. Therefore, the choice of length parameter may be made independently for each l -space, as b_l , and orthogonality of the basis of single-particle states will still be preserved. The considerations which enter the selection of the b_l values and the prescription used here are discussed further in [10].

T_{rel} is the Galilean-invariant relative kinetic energy operator

$$T_{\text{rel}} \equiv \frac{1}{4Am_N} \sum'_{ij} (\mathbf{p}_i - \mathbf{p}_j)^2 = \frac{1}{2Am_N} \left[(A-1) \underbrace{\sum_i \mathbf{p}_i^2}_{\text{one-body}} - \underbrace{\sum'_{ij} \mathbf{p}_i \cdot \mathbf{p}_j}_{\text{separable two-body}} \right]. \quad (3)$$

Here the prime on the summation \sum'_{ij} indicates $i \neq j$. This operator is seen to decompose into a one-body part and a separable two-body part. The Coulomb-Sturmian functions have a momentum-space representation $\tilde{S}_{nl}(b; k)$, where $p = \hbar k$, which is given simply in terms of a Jacobi polynomial [9, 15]. Matrix elements of the one-body term are readily evaluated as radial integrals of k^2 . Those of the two-body matrix elements factorize by Racah's reduction formula [17], as

$$\langle cd; J | \mathbf{p}_1 \cdot \mathbf{p}_2 | ab; J \rangle = (-)^{j_d + j_a + J} \begin{Bmatrix} j_c & j_d & J \\ j_b & j_a & 1 \end{Bmatrix} \langle c || \mathbf{p} || a \rangle \langle d || \mathbf{p} || b \rangle, \quad (4)$$

where each factor may again be evaluated in terms of a radial integral, more specifically, as $\langle b || \mathbf{p} || a \rangle \propto [\int_0^\infty dk \tilde{S}_{n_b l_b}(b_{l_b}; k) k \tilde{S}_{n_a l_a}(b_{l_a}; k)] \langle l_b j_b || Y_1 || l_a j_a \rangle$.

3. Calculations for ${}^6\text{Li}$

As a basic illustration of the use of the Coulomb-Sturmian basis for NCCI calculations, we now consider the nucleus ${}^6\text{Li}$. The code MFDn [18, 19] is used for the many-body calculations, taking as its input Hamiltonian two-body matrix elements obtained as outlined in section 2. The calculations are carried out for the JISP16 interaction [20].

The N_{max} truncation for the harmonic oscillator many-body basis is defined by the condition $N_{\text{tot}} \leq N_0 + N_{\text{max}}$, where $N_{\text{tot}} = \sum_i N_i = \sum_i (2n_i + l_i)$ is the total number of oscillator quanta, and N_0 is the minimal number of oscillator quanta for the given number of protons and neutrons. The calculated results depend both on the oscillator length parameter b — which is commonly quoted in terms of the oscillator energy $\hbar\Omega$, where $b = [\hbar/(m_N\Omega)]^{1/2}$, where m_N is the nucleon mass — and the truncation N_{max} for the basis. A natural question is how to truncate the Coulomb-Sturmian many-body basis, where a total number of oscillator quanta is not defined. However, we can *formally* carry over the N_{max} truncation scheme, if, for each Coulomb-Sturmian single-particle state, we simply define $N = 2n + l$ and, for each many-body state, we again define $N_{\text{tot}} = \sum_i N_i = \sum_i (2n_i + l_i)$. This choice of many-body truncation is certainly not unique, but it provides a reasonable starting point for further exploration, and it facilitates comparison of convergence rates obtained using the oscillator and Coulomb-Sturmian bases, since the dimensions of the many-body spaces are then the same in both cases.

First, let us review the conventional oscillator results for the energy of the 1^+ ground state, shown in figure 2(a). For any given choice of N_{max} , the energy has a variational minimum for some value of $\hbar\Omega$, ~ 20 MeV in this example. With increasing N_{max} , the ground-state eigenvalue approaches that for the infinite, untruncated space. The horizontal dashed line in figure 2 indicates the best extrapolation from prior calculations in an $N_{\text{max}} = 16$ space [21].

Calculations of the ground-state energy using the Coulomb-Sturmian basis are shown in figure 2(b). At each N_{max} the variational minimum energy obtained with the Coulomb-Sturmian basis in figure 2(b) is substantially higher than that obtained with the oscillator basis in figure 2(a). However, the energies obtained with the Coulomb-Sturmian basis are also falling significantly more rapidly with increasing N_{max} , and the quality of extrapolation appears to be comparable. We note that these exploratory results have not yet probed several variational freedoms available with the Coulomb-Sturmian basis, both in the length parameters b_l (see [10]) and in the many-body truncation scheme. The robustness of the many-body calculations against

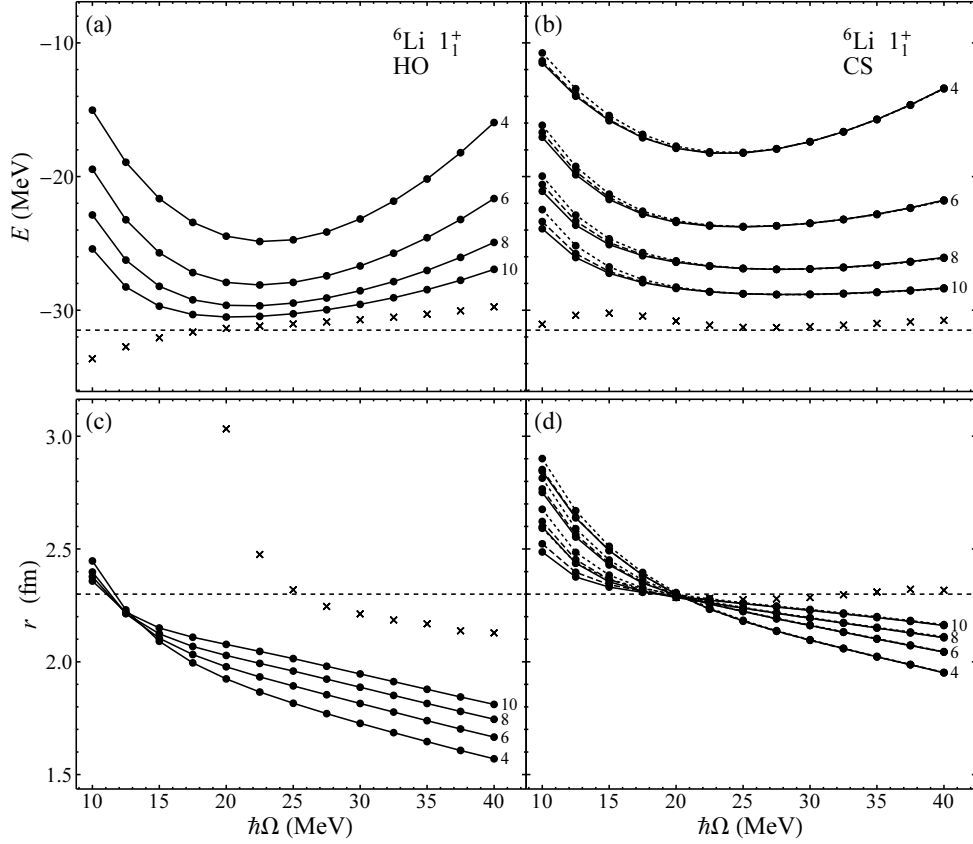


Figure 2. The ${}^6\text{Li } 1^+$ ground state energy, calculated using the conventional harmonic oscillator basis (left) and the Coulomb-Sturmian basis (right). Calculated energies (top) and RMS radii (bottom) are plotted as a function of the basis $\hbar\Omega$ parameter, for $N_{\text{max}} = 4, 6, 8,$ and 10 (successive curves, as labeled). For the Coulomb-Sturmian basis, calculations are shown variously for truncations $N_{\text{cut}} = 9, 11,$ and 13 (dotted, dashed, and solid curves, respectively). Exponentially extrapolated values are indicated by crosses. The best extrapolated values from the large-basis calculations of [21] are shown as horizontal dashed lines.

the truncation N_{cut} in the change-of-basis transformation (2) may also be verified from figure 2, where calculations based on two-body matrix elements obtained with $N_{\text{cut}} = 9, 11,$ and 13 are overlaid. The results for the ground state energy for $\hbar\Omega \gtrsim 20$ MeV are highly stable with respect to this cutoff. This range safely covers the variational minimum. If necessary, it would also be practicable to carry out transformations in larger oscillator spaces.

The root-mean-square (RMS) radius presents challenges for convergence in NCCI calculations with the conventional oscillator basis [22], since it is more specifically sensitive to the large- r asymptotic properties of the nuclear wavefunction. We compare the results obtained in the oscillator basis, shown in figure 2(c), with those obtained in the Coulomb-Sturmian basis, shown in figure 2(d). The extrapolated values obtained for $\hbar\Omega \gtrsim 20$ MeV, *i.e.*, above the crossover point, are reasonably insensitive to $\hbar\Omega$ and are consistent with the best estimate from large oscillator-basis calculations [21]. It would appear that the rate of convergence of the RMS radius obtained with the Coulomb-Sturmian basis is superior to that obtained with the conventional oscillator basis. However, further systematic investigation is required, especially into the stability of extrapolations with increasing N_{max} , before general conclusions may be drawn.

The dominant concern in using any basis other than the harmonic oscillator basis, with

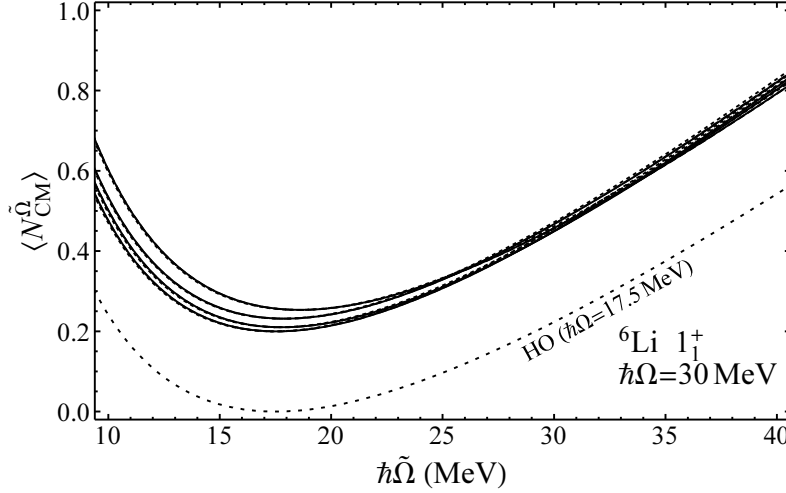


Figure 3. Expectation value of the number operator $N_{\text{c.m.}}^{\tilde{\Omega}}$ for center-of-mass oscillator quanta, as a function of oscillator energy $\hbar\tilde{\Omega}$. These calculations are for the ${}^6\text{Li } 1^+_1$ ground state, using the Coulomb-Sturmian basis, with $\hbar\Omega = 30$ MeV. Calculations are shown for $N_{\text{max}} = 4, 6, 8$, and 10 (successive curves, top to bottom), and for N_{cut} values as indicated in the caption to figure 2. The analogous curve expected for a pure harmonic oscillator 0s function, with $\hbar\Omega = 17.5$ MeV, is also shown (dotted curve, labeled).

N_{max} truncation, is incomplete separation of center-of-mass and intrinsic dynamics. There are several aspects to consider: the degree of separation arising in calculations using the Coulomb-Sturmian basis, the spurious state spectrum obtained in such calculations, and the extent to which a Lawson term [23] can be used to purge spurious excitations from the low-lying spectrum. Here we briefly discuss only the first consideration, *i.e.*, separation. However, it is also found that the spurious states are well-separated in the spectrum and are amenable to management with a Lawson term (see [10]).

A first indication of the degree of separation in the many-body eigenstate is provided by the expectation value of the number operator for center-of-mass harmonic oscillator quanta, defined for an arbitrary center-of-mass harmonic oscillator energy $\hbar\tilde{\Omega}$ by

$$N_{\text{c.m.}}^{\tilde{\Omega}} \equiv \frac{1}{\hbar\tilde{\Omega}} \left(\frac{P^2}{2Am_N} + \frac{Am_N\tilde{\Omega}^2 R^2}{2} - \frac{3\hbar\tilde{\Omega}}{2} \right), \quad (5)$$

where \mathbf{R} and \mathbf{P} are the center-of-mass coordinate and momentum, respectively. As noted by Hagen *et al.* [24], if separation occurs, as $\psi(\mathbf{r}_i; \boldsymbol{\sigma}_i) = \psi_{\text{c.m.}}(\mathbf{R})\psi_{\text{in}}(\mathbf{r}_{ij}; \boldsymbol{\sigma}_i)$, and if $\psi_{\text{c.m.}}(\mathbf{R})$ happens to be an oscillator 0s function, corresponding to some oscillator energy $\hbar\tilde{\Omega}$, then the many-body wavefunction will have $\langle N_{\text{c.m.}}^{\tilde{\Omega}} \rangle = 0$. The expectation value $\langle N_{\text{c.m.}}^{\tilde{\Omega}} \rangle$ is shown as a function of $\hbar\tilde{\Omega}$ for the ${}^6\text{Li}$ ground state in figure 3, for the Coulomb-Sturmian basis calculation with basis $\hbar\Omega = 30$ MeV and no Lawson term. The minimum of $\langle N_{\text{c.m.}}^{\tilde{\Omega}} \rangle$ is obtained at $\hbar\tilde{\Omega} \approx 17.5$ MeV. The minimum value decreases with increasing N_{max} , but it appears to be converging towards a *nonzero* $\langle N_{\text{c.m.}}^{\tilde{\Omega}} \rangle \sim 0.2$. The fact that expectation values significantly less than unity are obtained in the calculations indicates that a 0s oscillator function dominates the center-of-mass motion, and that an approximate separation of center-of-mass and intrinsic functions is spontaneously arising. However, the nonzero limit indicates that, as the full space is approached, the separated center-of-mass function is *not* strictly taking the form of a 0s oscillator function.

4. Summary

Although the conventional oscillator basis for the NCCI approach provides definite benefits, namely, exact center-of-mass factorization in the N_{max} truncation and the simplicity of the Moshinsky transformation for generating two-body matrix elements, it also exhibits nonphysical Gaussian asymptotics at large distances. The Coulomb-Sturmian functions form a complete, discrete set of square-integrable functions with realistic exponential asymptotics. A principal goal in using such a basis is to obtain improved convergence of observables which are sensitive to the asymptotics, such as RMS radii and $E2$ matrix elements. Such a basis might be particularly appropriate to halo nuclei, where the mismatch with the oscillator functions at large distances is particularly severe. The computational framework for the many-body calculation has the standard structure for an nlj single-particle basis, and the interaction matrix elements are transformed from the harmonic-oscillator basis, except that relative kinetic energy matrix elements (and, in fact, those for $N_{\text{c.m.}}$ and r^2 , as well) are calculated directly in the Coulomb-Sturmian basis. The initial exploratory calculations considered here indicate that convergence properties are promising. Moreover, the spurious center-of-mass dynamics are found to be tractable.

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